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Local effective viscosity of gas in nano-scale channels

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ABSTRACT

The non-equilibrium molecular dynamics method is used in the present study to investigate the local effective viscosity in nano-scale shear-driven gas flows. The profiles of gas velocity and shear stress across the channel are sampled and the Newton law of viscosity is applied to obtain the local effective viscosity. By using this method, the profile of local effective viscosity across the channel is obtained. In the bulk region of the channel, the local effective viscosity agrees well with the experimental value. However, in the near wall region, the local effective viscosity deviates from experimental value. The wall influence depth decreases with the increase of gas density, and this depth is independent of channel height, temperature and shear velocity in the shear driven Couette flow. The wall influence depth is approximately twice of the mean free path.

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1. Introduction

With the rapid development of nanotechnology, nano-electro-mechanical systems have received great attentions during the past decade. Many of these systems are engaged with fluid flow phenomena, e.g., motors, actuators, sensors, and valves [1,2]. Understanding the flow of fluid at the nano-scale is currently a subject of great interest [3–8].

Extraordinarily fast transport of fluid in carbon nanotubes (CNTs) are discovered in many experimental investigations. Pressure driven flow velocities of 4 or 5 orders of magnitude higher than predicted from Newtonian flow using the Hagen–Poiseuille equation have been observed in multi-walled carbon nanotube membrane pores of 7 nm inner diameter by Majumder et al. [9]. In double walled carbon nanotube pores with an inner diameter of 1.6 nm, Holt et al. [10] found that the measured water flow exceeds values calculated from continuum hydrodynamics models by more than 3 orders of magnitude. For flows of water, ethanol, and decane through carbon nano-pipes with inner diameters of 43 nm, Whitby et al. [11] found enhanced transport up to 45 times theoretical predictions.

Molecular dynamics (MD) simulations are also employed by many researchers to study the fluid flow behaviors in CNTs or nano-channels and much greater flow rate than expected has also been discovered, for both liquid and gas flows [12–17]. This enhanced flow in CNTs or nano-scale channels is considered to be

a result of the low friction in the channel [9,14]. Hence, it would be of great interest to investigate the fluid viscosity in nano-scale channels.

Fichman and Hetsroni [18] analyzed the effective gas viscosity in Knudsen layer in nano-scale channel. They found that the effective gas viscosity is lower in comparison with the viscosity in the bulk fluid, because of the interaction between wall and fluid molecules. Based on the analytical relations given for the viscosity coefficient at the two limits of continuum and free molecular regimes, Karniadakis et al. [3] found that the viscosity decreases with the increase of rarefaction. From the distribution of the mean free path near the wall, Dongari et al. [19] found that the gas viscosity decreases when approaching the wall, obeying power-law. Lockerby et al. [20] investigated the applicability of higher-order continuum equations to model the Knudsen layer, and compared their predictions to high-accuracy DSMC. Fei et al. [21] analytically investigated the viscosity of gas confined between two parallel solid walls using the Green–Kubo relation [22,23] with the hard-sphere model. They found that the average viscosity decreases with the decrease of distance between two walls. But up to now, most researchers concerned with the average viscosity in nano-channels.

Direct measurement of fluid viscosity in a nano-channel is beyond present experimental technology [24]. However, an MD simulation provides an insight at the atomic level and is the most appropriate method to investigate the shear viscosity at nano-scale [25]. The shear viscosity in MD simulation can be calculated through equilibrium MD (EMD) or non-equilibrium MD (NEMD) simulations. In EMD simulation, Green–Kubo formula [22,23], which relates shear viscosity to off-diagonal components

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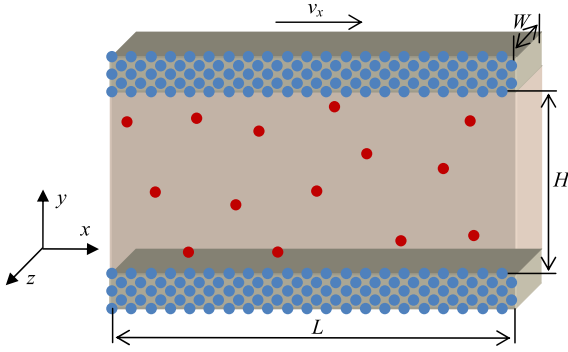


Fig. 1. Schematic of shear-driven Couette flow.

of pressure tensor, is widely used to calculate the shear viscosity in systems close to or in equilibrium state. This approach entails integration over all distances and time, which leads to cumbersome calculations due to long time tails [26]. The viscosity can also be derived from the Einstein relation via self-diffusion constant, which may also employ the Green–Kubo formula for velocity–velocity time correlation functions. In NEMD simulation, a possible approach is to calculate shear viscosity from direct, non-equilibrium simulations of Couette flow, *i.e.* pure one-dimensional shear flow. Modeling the flow of the atoms characterized by the uniform transverse velocity gradient under pure shear tension leads to direct determination of the shear viscosity [26]. In systems confined between solid walls, if one takes into account the induced strain rates, NEMD methods for the calculation of shear viscosity are a good alternative.

Sofos et al. [27] investigated the shear viscosity of liquid argon in nano-scale channels by NEMD simulation. They found that fluid layers close to the walls always present distinctly different behavior due to the interaction with the wall atoms. Furthermore, they observed a critical dimension, in the range 7–18 σ , below which the shear viscosity deviates from the bulk value [28].

But up to now, seldom investigations on the local viscosity in nano-scale channels can be found in the literature. The objective of this study is to investigate the local effective viscosity in nano-scale channels, and to reveal the scale effect of effective viscosity. This paper is organized as follows: in Section 2, the MD simulation is introduced; the local effective viscosity profiles in nano-channels and wall influence depths are discussed in Section 3; and finally, Section 4 concludes the present study.

2. Molecular dynamics simulation

Without losing generality, argon gas confined between two platinum walls, which are a distance H apart is investigated, as illustrated in Fig. 1. The wall atoms are frozen, and the thicknesses of both walls are 0.98 nm, which is larger than the fluid–wall interactional cut-off radius, r_c . The platinum wall is consist of Face-Centered Cubic (FCC) lattice, and the lattice constant is 0.392 nm. The bottom wall is stationary, while the upper wall moves with a specified velocity, v_x . The simulation box is periodic in the x and z directions.

The interactions between fluid–fluid and fluid–wall molecules are both described by the truncated and shifted Lennard-Jones (LJ) 12-6 potential, given as:

$$V(r_{ij}) = \begin{cases} 4\epsilon \left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^6 - \left(\frac{\sigma}{r_c}\right)^{12} + \left(\frac{\sigma}{r_c}\right)^6 \right] & r_{ij} \leq r_c \\ 0 & r_{ij} > r_c, \end{cases} \quad (1)$$

where r_{ij} is the intermolecular distance between molecules i and j , ϵ is the depth of the potential well, σ is the molecular diameter, and r_c is the cut-off radius. In the present study, argon is employed as fluid molecule. The diameter, σ_{Ar} , and potential depth, ϵ_{Ar} , of argon are 0.3405 nm and 119.8 k_B , respectively. While for the argon–platinum molecular interaction, σ_{Ar-Pt} is 0.3085 nm and ϵ_{Ar-Pt} is 64.8 k_B [29]. r_c is chosen to be 0.851 nm, which is approximately 2.5 σ_{Ar} .

In the present study, the simulation box is divided into different bins in the y direction. The height of each bin, dH , is chosen to be 0.05 nm, which is small enough to characterize flow variations. This bin height remains the same in all simulations. Shear viscosity is then evaluated as a local value in each bin. As a result, shear viscosity varies in the y -direction. For a pure fluid, shear viscosity can be computed using:

$$\mu(y) = -\frac{\langle P_{xy}(y) \rangle}{\dot{\gamma}(y)}, \quad (2)$$

where $P_{xy}(y)$ is the off-diagonal component of the microscopic stress tensor \mathbf{P} , and $\langle \cdot \cdot \cdot \rangle$ denotes time-averaged values. P_{xy} is given by [30]

$$P_{xy} = \frac{1}{V_{bin}} \left(\sum_{i=1}^N m_i v_{xi} v_{yi} - \sum_{i=1}^N \sum_{j>i}^N r_{ij} F_{ij} \right), \quad (3)$$

where r_{ij} is the distance between atoms i and j , and v_{ji} is the j -component ($j = x, y$ or z) of the velocity of atom i (the mean flow velocity is subtracted). V_{bin} is the volume of each bin, and $V_{bin} = L \times W \times dH$. The above expression for the stress tensor can be divided into a kinetic and a potential energy part.

The strain rate $\dot{\gamma}_{xy}$ is:

$$\dot{\gamma}_{xy} = \frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x}. \quad (4)$$

For flat channel walls, the second term on the right of Eq. (4) is negligible, thus the first term on the right of Eq. (4) is dominant and taken into account in the simulations.

In our simulations, the neighbor-list method is used to calculate the force between atoms while the velocity-Verlet algorithm is adopted to integrate the equations of motion [31]. The time step in the simulation is set to be 10.8 fs. The first 1 million steps are used to equilibrate the system and another 5 million steps are used to accumulate properties. The Langevin thermostat method [32] is employed to control the gas temperature before equilibrium. Only thermal velocities are used to compute the temperature and pressure.

3. Results and discussions

3.1. Local effective viscosity

The gas Couette flow in a typical channel is investigated firstly. The channel height is 150 nm. Since the simulation box is periodic in the x and z directions, L and W are chosen both 40 nm in the simulation. The lower wall is stationary and the fluid is driven by the moving upper wall, with a velocity of 473.7 m/s. 30 870 argon molecules and 105 063 platinum atoms are employed in the simulation. The initial density of gas is 8.45 kg/m³ and gas temperature is kept at 300 K, using Langevin thermostat method [32]. The gas pressure is 0.527 MPa. According to the definition,

$$\lambda = \frac{1}{\sqrt{2}\pi n d^2}, \quad (5)$$

the mean free path of argon gas is 15.33 nm. The Knudsen number, defined as the ratio of gas mean free path to channel height, is 0.102. The gas flow is in early transition regime.

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